Nano-mechanical Processing of Quantum Information with Lithium Atoms in Silicon

Support:

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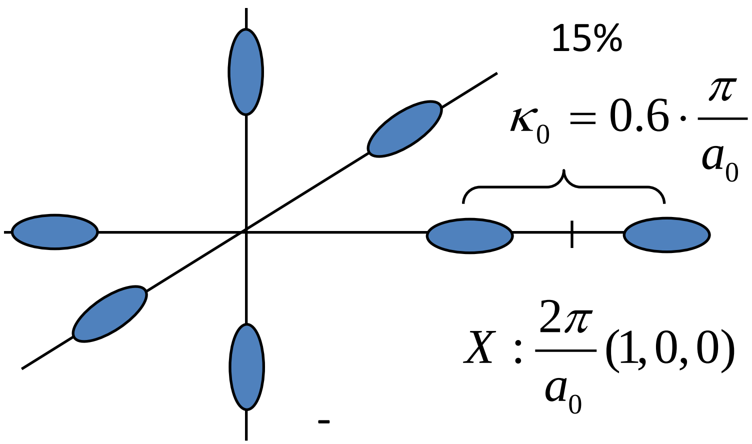
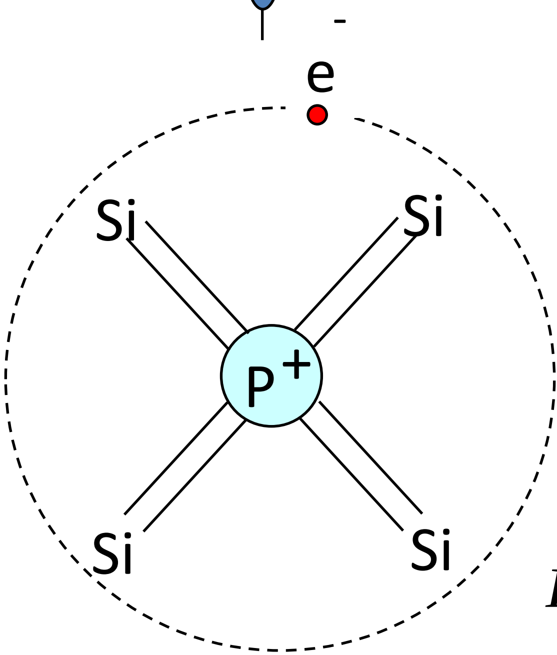
The interstitial lithium donor in silicon is unique amongst shallow donors because it has an inverted level structure and a degeneracy within the 1s ground state manifold. The latter gives rise to a strong long-range elastic-dipole coupling of the neutral Li donor orbital states, similar to that obtained earlier for acceptors in Si by Golding and Dykman but absent in the case of other donors. This coupling can be used for a quantum computing architecture based on the stress-defined orbital qubits in lithium donors in silicon. The above interaction can be used to enable 2-qubit gates while individual qubit control can be done by a resonant excitation of acoustic waves. At the same time the near degeneracy of 1s manifold in lithium donor in silicon also gives rise to a nontrivial coupling between the spin and orbital degrees of freedom first investigated by Watkins and Ham. One can expect that the inverted level structure and near degeneracy in 1s manifold will lead to a very short electron spin relaxation times which can also strongly affect orbital relaxation and be detrimental for QIP. Somewhat surprisingly, in view of extensive studies of spin relaxation of other shallow donors in silicon since the early sixties, both experimental and theoretical, the question about Li spin relaxation has not been addressed. We investigate the lithium spin relaxation in ESR and FTIR experiments as well as control of individual qubits and 2-gate operations.

Substitutional donors in Si

Effective mass theory (EMT), Kohn & Luttinger, 1955





Length and energy scales:

$$a_{\perp,\parallel} = \frac{\varepsilon \hbar^2}{m_{\perp,\parallel} \cdot e^2}, \quad Ry^* = \frac{m_\perp e^4}{2\hbar^2 \varepsilon^2}, \quad \gamma = \frac{a_\parallel}{a_\perp}$$

$$a_\perp = 2.34\,\text{nm} \qquad a_\parallel = 1.35\,\text{nm}$$

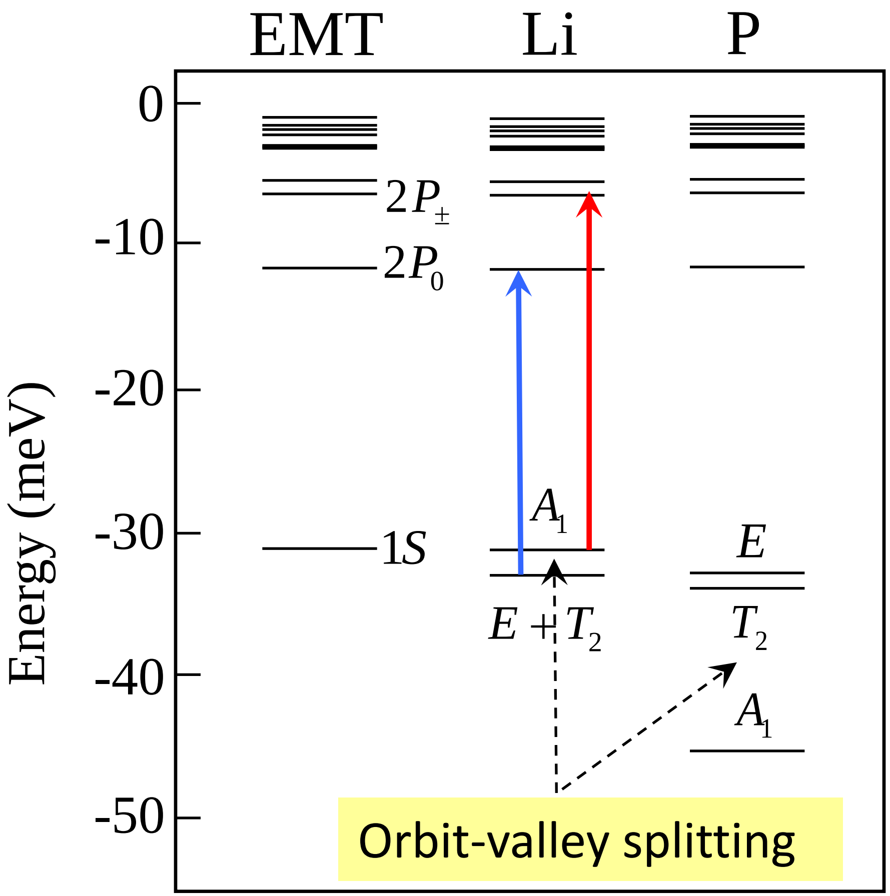
Dimensionless Hamiltonian:

$$H_0 = -\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \gamma \frac{\partial^2}{\partial z^2} \right) - \frac{2}{r}$$

1s envelope function:

$$F_{1s}^z(\mathbf{r}) = \left(\frac{1}{\pi a_\perp^2 a_\parallel} \right)^{1/2} \exp\left[-\sqrt{\left(x^2 + y^2\right)/a_\perp^2 + z^2/a_\parallel^2} \right]$$

Non-EMT corrections: valley-orbit splitting



$$\Psi^{\mu}(\vec{r}) = \sum_{j=1}^{6} \alpha_{\mu,j} F_{\mu}^{j}(\vec{r}) \psi_{\vec{k}_j}(\vec{r})$$

Irreducible representations of T_d –symmetry group

$$(x, -x, y, -y, z, -z)$$

$$\alpha_{A_1,j} = 6^{-1/2}(1,\ 1,\ 1,\ 1,\ 1,\ 1) \quad \text{even}$$

$$\alpha_{T_2,j} = \begin{cases} 2^{-1/2}(1,-1,0,0,0,0) \\ 2^{-1/2}(0,0,1,-1,0,0) \\ 2^{-1/2}(0,0,0,0,1,-1) \end{cases} \quad \text{odd}$$

$$\alpha_{E,j} = \begin{cases} 12^{-1/2}(-1,-1,-1,-1,-1,2,2) \\ 2^{-1}(1,1,-1,-1,0,0) \end{cases} \quad \text{even}$$

Interstitial Li:

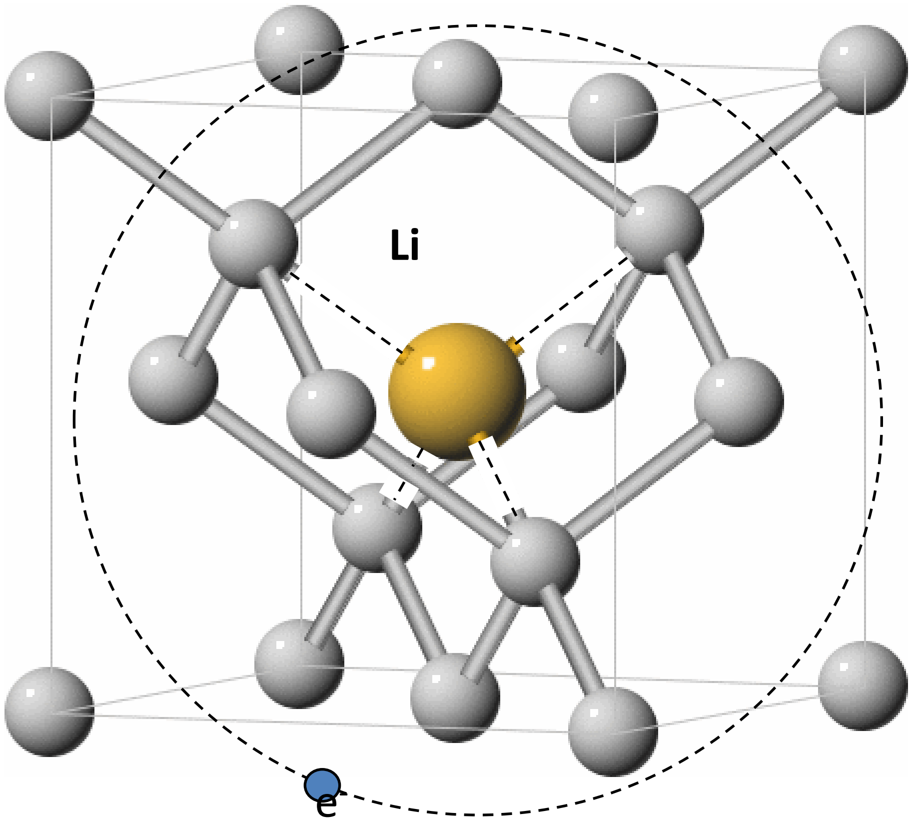
- Degenerate ground state
- Inverted sequence of levels

Interstitial donor Li in Si

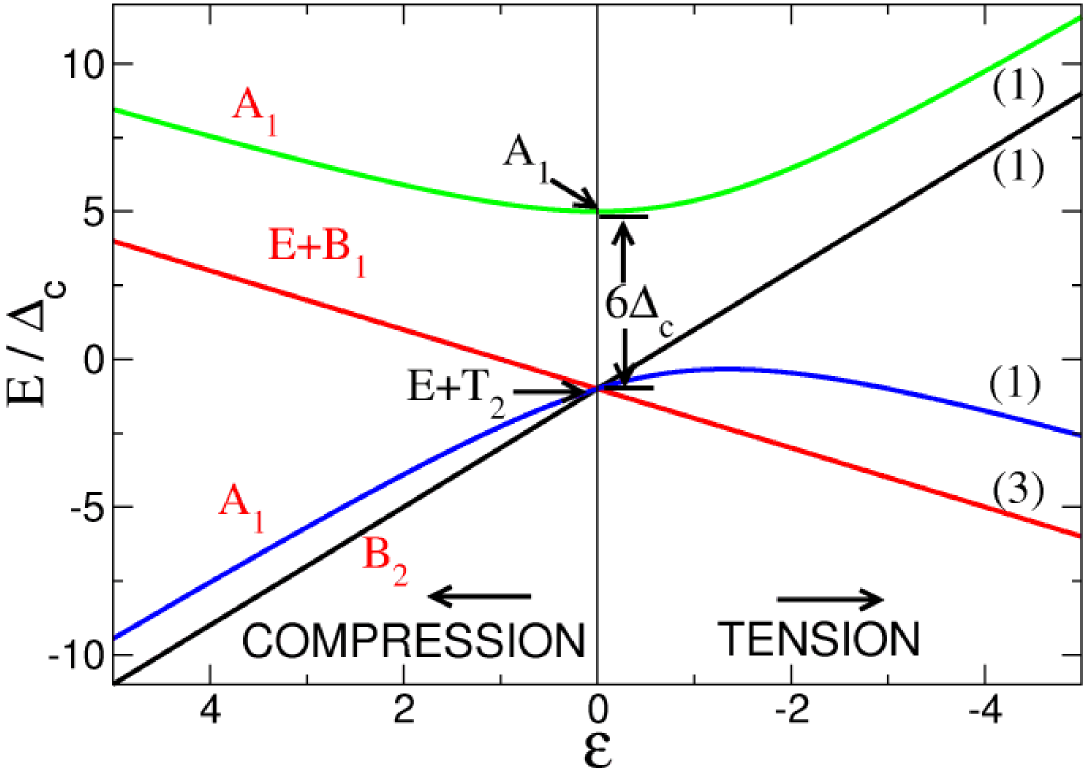
$1s^2 2s$

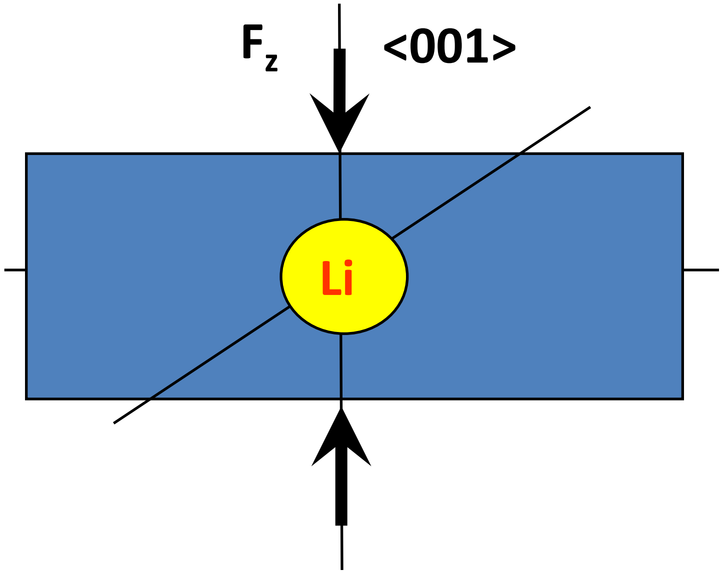
- **interstitial impurity**
- **local symmetry the same as in substitutional donors**
- **weak, repulsive central cell potential**

T_d site symmetry



Si:Li spectrum under uniaxial stress





$$\Delta_0 = 6\Delta_c = 1.76 \;\; \text{meV}$$

$$\varepsilon = (3\Delta_c)^{-1}\Xi_u(s_{11} - s_{12})F_z$$

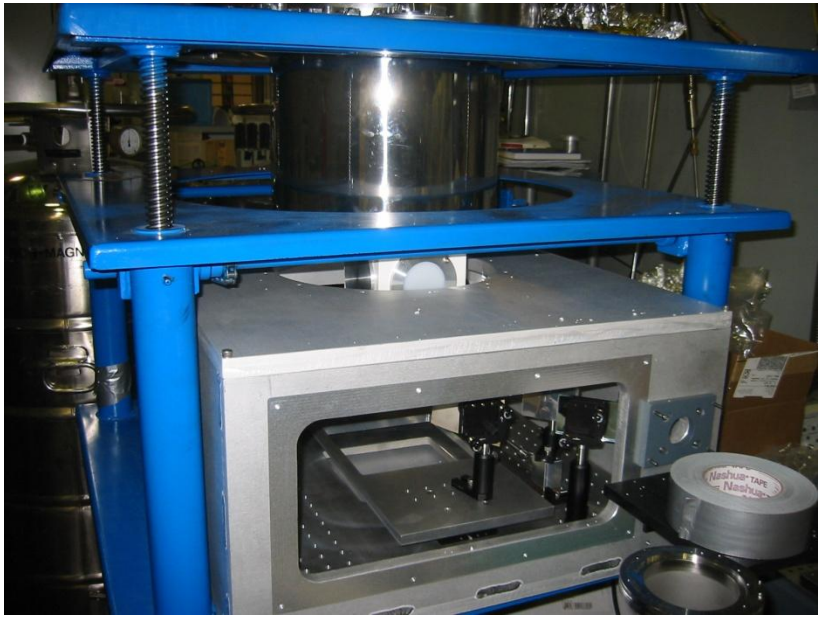
Stress-defined qubit states

$B_2 \quad \alpha = (0,0,0,0,1,-1)/\sqrt{2} \Rightarrow |0\rangle$ parity odd

$A_1 \quad \alpha = (a,a,a,a,b,b) \Rightarrow |1\rangle$ parity even

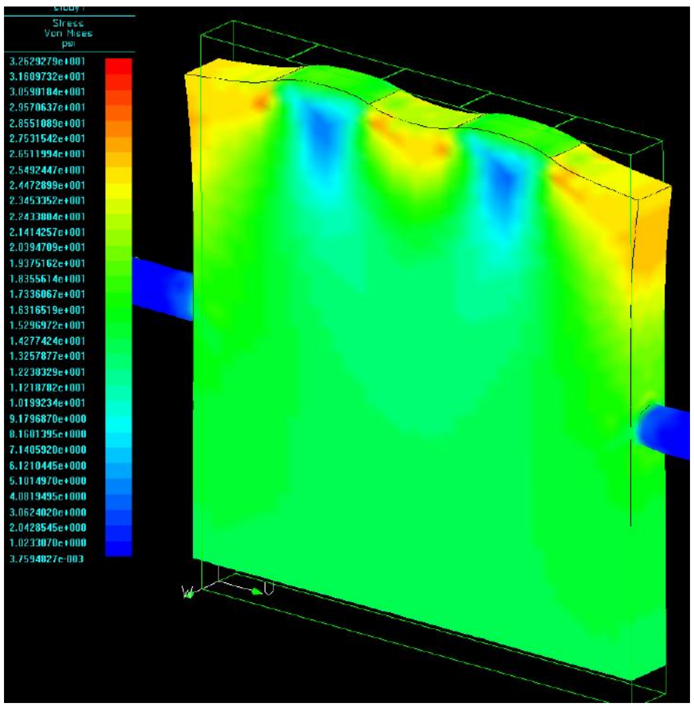
FTIR to probe stress excited Li in Si

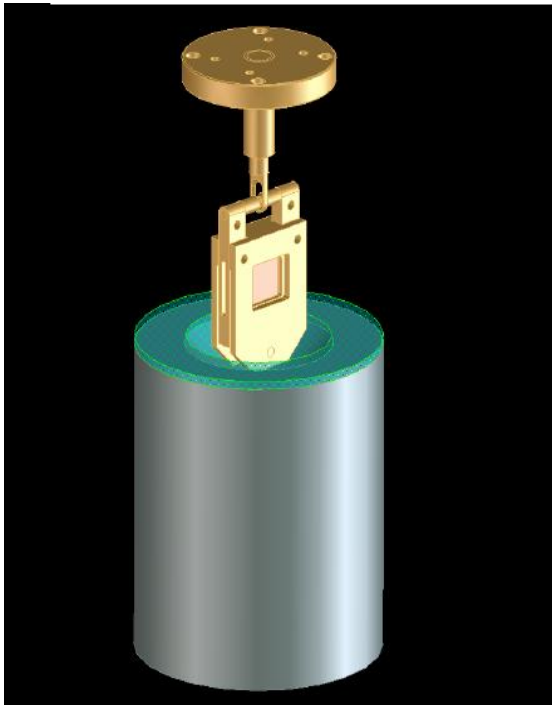
experiments at ALS, collaborators. M. Martin and Z. Hao

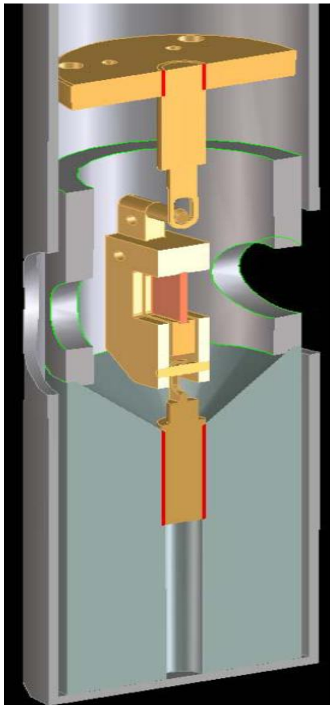


optics box for coupling of He-3 cryostat
to FTIR spectrometer

Design of sample holder with Stress in a static Magnetic Field for FTIR in the He-3 cryostat







- calculations of stress distribution across LiSi sample

- model for stressed sample holder compadible with tight He-3 dimensions

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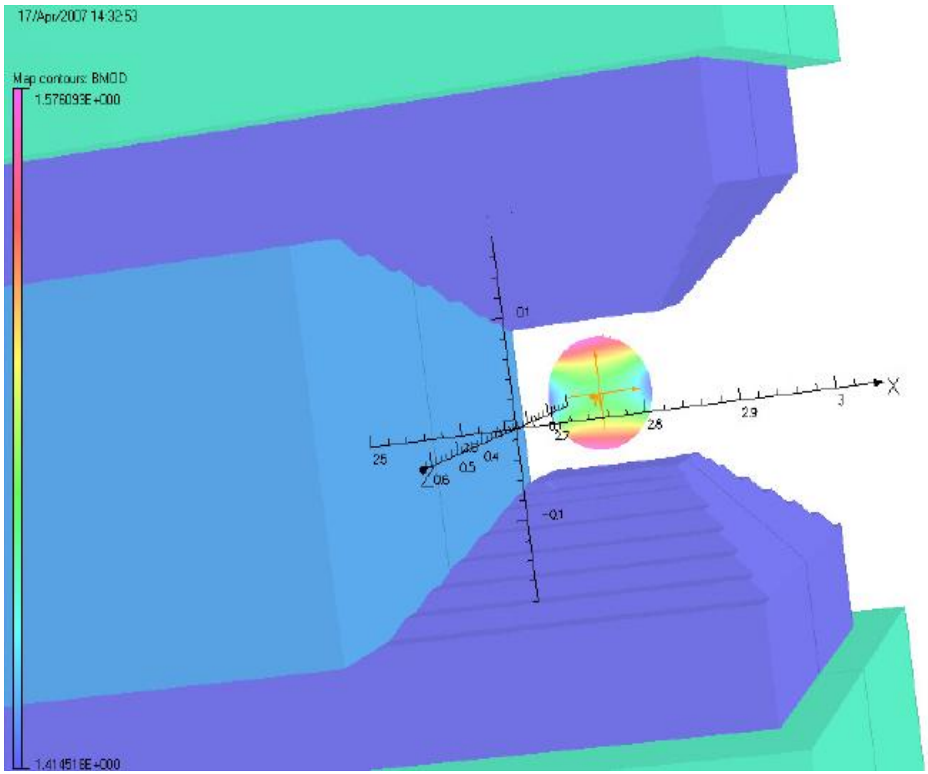
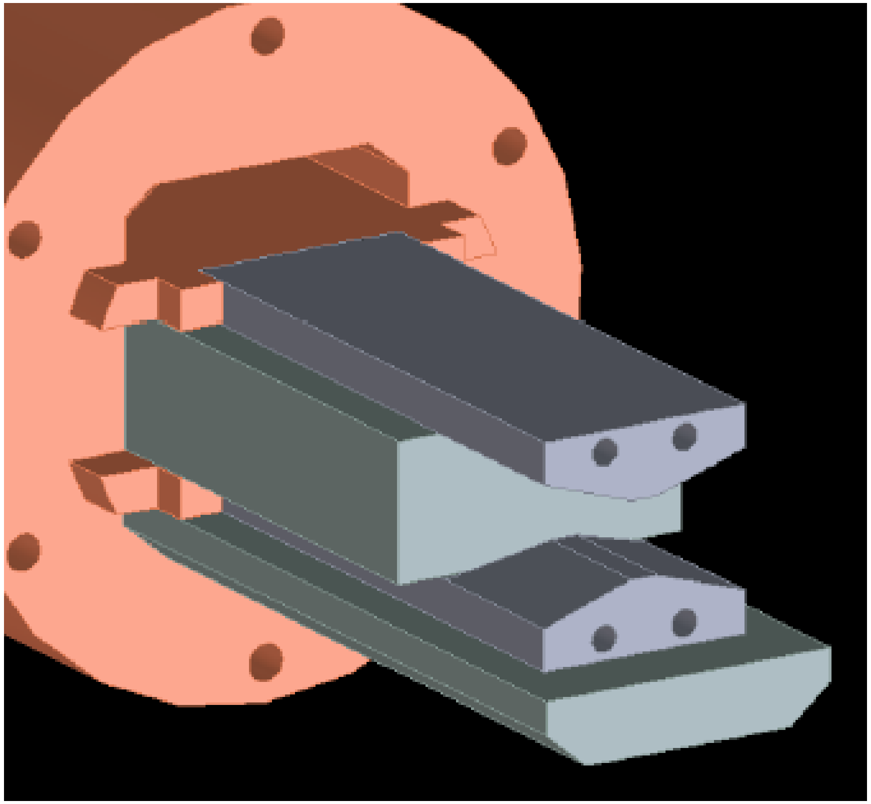
Design of FIR accessible sampel holder with stress and static magnetic field (homogeneous, 0.6 T) for He-3 system





• have design of a homogeneous hybrid magnet with 0.6 T strength and low temperature compadibility, need to modify LHe shield in the He-3 cryostat, fabricate and test the holder with magnetic field and stress

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First-principles charge density on Si:Li donor